Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Wang-Landau sampling of protein adsorption using the HP model[1] YING-WAI LI, D.P. LANDAU, Center for Simulational Physics, University of Georgia, T. WUEST, Swiss Federal Research Institute — We have applied Wang-Landau sampling[2] with appropriate trial moves[3] to investigate the thermodynamics and structural properties of lattice hydrophobic-polar heteropolymers (commonly known as the HP protein model) interacting with an attractive substrate. We estimate the density of states of the system, from which the partition function and all thermodynamic quantities, e.g. specific heat, radius of gyration, end-to-end distance and surface contacts, can be calculated. "Transitions" between "phases" are then identified based on a comprehensive analysis of these observables. Generally speaking, three transition processes are observed: adsorption-desorption, collapse (formation of hydrophobic core), and "flattening" of adsorbed structures. These have been confirmed by "snapshots" of typical states of the system. Depending on the surface attractive strength, these transitions take place in different order upon cooling, giving rise to different thermodynamic behaviors. Such dependence of folding hierarchy on the surface attraction is found to be universal for different HP sequences.

[1]Research supported by NSF.
[2]F. Wang and D. P. Landau, Phy. Rev. Lett. **86**, 2050 (2001).
[3]T. Wüst and D. P. Landau, Phy. Rev. Lett. **102**, 178101 (2009).

Ying-Wai Li
Center for Simulational Physics, University of Georgia

Date submitted: 09 Nov 2010 Electronic form version 1.4